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The Partial Donor Cell Method

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The partial donor cell method is a nonlinear combination of the donor cell method and a second order scheme. It prevents the appearance of maxima or minima caused by the higher order scheme. The dependent variable is stationary for zero velocity and the method can readily be generalized to multidimensions.

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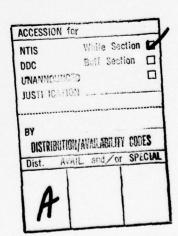
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THE PARTIAL DONOR CELL METHOD

I. Introduction

The use of second order or higher interpolation schemes for convection terms causes the appearance of unwanted extremes near points where the transported function changes its slope rapidly. donor cell method uses first order interpolation and therefore cannot generate such extrema, but it has a diffusion which is unacceptable in most cases. The partial donor cell method (PDM) presented here is nonlinear combination of a higher order scheme and the donor cell method. It adds just enough diffusion to prevent the occurrence of such extrema. As compared with other hybrid methods it is less diffusive because it restricts the additional diffusion to points where it is absolutely necessary. Flux-Corrected Transport (FCT), on the other hand, removes the extrema after they have occured. The results of this method and FCT are very similar, as demonstrated in the test runs. The PDM leaves the solution undisturbed for zero velocities. It therefore cannot be used to create artificial viscosity in stationary or nearly stationary shock fronts. The method can be readily extended to multidimensions.

II. Theory

Let f be the function to be transported across a one-dimensional grid; we denote by f; the value of the function at x;. Furthermore, let d be the difference operator,

$$df_{j+1/2} = f_{j+1} - f_{j}.$$
 (1)

Note: Manuscript submitted January 30, 1978.

Two higher-order schemes are considered here.

a) A simple scheme.

Let all quantities be defined at integral points at space and time, with the exception of the velocity u, defined at half integral points in space and time. Then, the new value of f_j is given by

$$\hat{f}_{j} = f_{j} - \frac{dt}{2} (u_{j+1/2} (f_{j+1} + f_{j}) - u_{j-1/2} (f_{j} + f_{j-1})) / dx_{j+1/2}$$
 (2)

The scheme is unstable, with an amplification factor

$$A = 1 + 1/2 \left(\frac{u dt}{dx}\right)^2.$$

The addition of a second order term, corresponding to a second order interpolation, will make this scheme stable.

b) Lax-Wendroff Scheme.

In this scheme, one defines intermediate values as

$$f_{j+1/2} = 1/2(f_j + f_{j+1}) - \frac{dt}{2} (u_{j+1} f_{j+1} - u_j f_j)/dx_{j+1/2}$$
 (3)

then, with $\hat{u}_{j+1/2}$ defined similarly

$$\hat{f}_{j} = f_{j} - dt (\hat{u}_{j+1/2})^{2} \hat{f}_{j+1/2} - \hat{u}_{j+1/2})^{2} \hat{f}_{j-1/2} / dx_{j}$$
 (4)

The donor cell method can be written in the form

$$\hat{f}_{j} = f_{j} - \frac{dt}{2} (1 - sign(u_{j})) f_{j+1} u_{j+1} - f_{j}u_{j})/dx_{j+1/2}$$

$$(1 + sign(u_{j})) (f_{j}u_{j} - f_{j-1} u_{j-1})/dx_{j-1/2}$$
(5)

or

$$\begin{split} \hat{f}_{j} &= f_{j} - \frac{dt}{2} \left[(f_{j+1} u_{j+1} - f_{j} u_{j}) / dx_{j+1/2} + (f_{n} u_{j} - f_{j-1} u_{j-1}) / dx_{j-1/2} \right] \\ &+ \frac{dt}{2} \operatorname{sign}(u_{j}) \left[(f_{j+1} u_{j+1} - f_{j} u_{m}) / dx_{j+1/2} - (f_{j} u_{j} - f_{n-1}) / dx_{j-1/2} \right]^{(5a)}. \end{split}$$

As is well-known, the difference between the donor cell method and the simple scheme (a) defined above is a diffusion term (the second term in equation 5a) first order in time and second order in space.

(The difference in the case of the Lax-Wendroff scheme also involves a higher order term in space and time.)

In order to derive the partial donor cell method, let us define for the scheme (a)

$$\varepsilon_{j+1/2} = 1/2 \text{ dt } | u_{j+1/2} | / dx_{j+1/2},$$
 (6)

and for scheme (b)

$$\varepsilon_{j+1/2} = 1/2 \text{ dt } | u_j^{+1/2} | /dx_{j+1/2} (1 - dt | u_{j+1/2} | /dx_{j+1/2})$$
 (6a)

Furthermore, let $\sigma_{j+1/2}$ be an array of numbers such that

$$\sigma \leq \sigma_{j+1/2} \leq 1;$$

here σ represents the fraction of diffusion to be added. If σ = 1, the complete donor cell method would result. It should be emphasized, however, that this holds for variable velocities only up to terms second order in time and third order in space.

With these definitions, we add the following diffusion terms in a conservative manner to either the simple scheme or the Lax-Wendroff scheme:

$$D_{j} = \epsilon_{j+1/2} \quad \sigma_{j+1/2} \quad df_{j+1/2} - \epsilon_{j-1/2} \quad \sigma_{j-1/2} \quad df_{j-1/2}$$
 (7)

In order to simplify the following discussion let us assume for a moment constant velocity and $\mathbf{u} > 0$, and discuss only the simple scheme. Then with

$$\varepsilon = u \, dt/dx$$

we can rewrite the transport algorithm including diffusion as

$$\hat{f}_{j} = f_{j} - \frac{\varepsilon}{2} (f_{j+1} - f_{j-1}) + \frac{\varepsilon}{2} (\sigma_{j+1/2} df_{j+1/2} - \sigma_{j-1/2} df_{j-1/2}), (8)$$

or setting

$$\mu_{j+1/2} = \sigma_{j+1/2} df_{j+1/2},$$
(9)

$$\hat{f}_{j} = f_{j} - \frac{\varepsilon}{2} (f_{j+1} - f_{j-1}) + \frac{\varepsilon}{2} (\mu_{j+1/2} - \mu_{j-1/2}).$$
 (10)

The main question is how to determine μ . As the convection is nothing but an interpolation between x_j and x_{j-1} (for u>0), the new value of the function must lie between f_j and f_{j-1} . This implies if f_j is not an extrema in the absence of diffusion that

$$\frac{\varepsilon}{2} \mid f_{j+1} - f_{j-1} \mid < |f_j - f_{j-1}|.$$

If this is not the case, some diffusion has to be added to make the updated function value lie between these limits. The diffusion depends obviously on the direction in which the fluid moves and therefore should incorporate this information. One way to take it into account is the following. Let us define

$$S_{j} = A + \frac{B}{2} | sign(df_{j+1/2}) + sign(df_{j-1/2}) |;$$
 (11)

then we write $\mu_{j+1/2}$ in general in the form

$$\mu_{j+1/2} = \text{sign } (df_{j+1/2}) \max \left[0, |df_{j+1/2}| \right]$$

$$-1/2 S_{j+1} (1 - \text{sign } (u_{j+1/2})) | df_{j+3/2}|$$

$$-1/2 S_{j} (1 + \text{sign } (u_{j+1/2})) | df_{j-1/2} | \right].$$
(12)

This prescription means we subtract df, the difference $\mathrm{df}_{j+1/2}$ taken in the direction of the flow, the amount A whether or not the function has an extremum at this point, and the amount B only if there is no extremum. But, if the amount exceeds the difference $\mathrm{df}_{j+1/2}$ no diffusion will result. This is the point where (as in FCT) the nonlinearity comes in. The values of A and B remain to be determined.

In order to relate this diffusion to the hybrid schemes described by Harten 2 and Van Leer 3 we define a quantity θ by

$$\theta_{j} = \frac{\left| df_{j+1/2} \right| - \left| df_{j-1/2} \right|}{\left| df_{j+1/2} \right| + \left| df_{j-1/2} \right|}$$
(13)

(compare Eq. 4.12a, 4.12b of ref. 2). Harten's method then can be written in our notation as

$$\mu_{j+1/2}^{H} = \max (\theta_{j}, \theta_{j+1}) df_{j+1/2}$$
 (14)

This means the solution has an added diffusion proportional to this smoothness parameter θ_j . In order to make the connection with our methods more obvious, let us define

$$\theta_{j}^{+} = \max (0, |df_{j+1/2}| - S_{j} |df_{j-1/2}|)/|df_{j+1/2}|;$$
 (15a)

$$\theta_{j}^{-} = \max (0, |df_{j-1/2}| - s_{j} |df_{j+1/2}|)/|df_{j-1/2}|.$$
 (15b)

With these definitions we can rewrite Eq. (12) as

$$\mu_{j+1/2} = df_{j+1/2} \frac{1}{2} \left[(1 - sign (u_{j+1/2})) \theta_{j+1} + (1 + sign (u_{j+1/2})) \theta_{j}^{+} \right]$$

$$(16).$$

The choice of A = 1, B = 0, therefore, closely resembles the hybrid scheme of Harten and Van Leer.

The important difference is that in the partial donor cell method only as much diffusion is added as is needed to keep the function f monotone. This is achieved in two ways; first, by considering only the differences in the direction from which the fluid comes; second, by taking the maximum in Eqs. (15). The possibility of adjusting the parameters A and B is a further advantage.

We now discuss the manner in which A and B are determined. The simplest argument, which leads to A = 0 and B = 1, is the following. If

$$1/2 \mid f_{j+1} - f_{j-1} \mid \leq \mid f_{j} - f_{j-1} \mid$$

then no extrema can occur. That is, if f_i has no extrema, this is equivalent to

$$| f_{i+1} - f_{i} | \le | f_{i} - f_{i-1} |$$

Therefore, no additional diffusion is needed implying A + B = 1.

The choice of linear interpolation at all extrema leads to A = 0. A more sophisticated argument proceeds as follows. It is presented here for scheme a: if f_{ij} is not an extreme and as long as

$$\frac{\varepsilon}{2} \mid f_{i+1} - f_{i-1} \mid \leq \mid f_i - f_{i-1} \mid$$

the new values lie between f_j and f_{j-1} . Furthermore, at an extremum interpolation with a symmetric parabola will not result in a new extremum. Therefore, the value A = 1 can be chosen. If the signs of the differences do not change, the condition above leads to

$$|f_{j+1} - f_j| < (\frac{2}{\epsilon} - 1) |f_j - f_{j-1}|.$$

If one chooses B such that only additional diffusion is added if this condition is not satisfied, namely (similar for b))

a)
$$B = \frac{2}{\varepsilon} - 2$$
, b) $B = \frac{2}{\varepsilon}$

then at points where the subtracted difference is smaller, $f_j = f_{j-1}$ regardless of the value of ϵ . This leads to great phase errors locally. A good choice is to take the values found for $\epsilon = 1/2$. The results for the two schemes are

a)
$$A = 1$$
 b) $A = 1$ $B = 2$

(One should remark that usually in hydrodynamics ϵ at its maximum is about 0.3; therefore, the phase errors should not be too big.) This choice assures the correct range of f_j . The test runs confirm also that it is less diffusive than the choice A=0, B=1. The results are for all practical purposes identical with those of FCT for the transport of square waves. Test runs with rapid varying velocity have shown that the best results were achieved with A=0, B=1. A description of this algorithm is given in Appendix B.

Test runs:

Test runs have been done for three cases:

- 1) Squarewave 10 meshpoints across.
- 2) Squarewave two meshpoints across.
- 3) Cosine wave with 10 points for the total period. For the choice ϵ = .2, the results are presented at 10 and 100 steps, for which the solution is propagated 2 and 20 mes. oints, respectively. The results are given in the tables below (tables were chosen because of the small differences). One sees clearly that for all the test A = 0, B = 1, is most diffusive, but gives basically the same results. The choice of A = 1, B = 2 in the 10 point square wave yields the same results as does FCT (as described in the appendix). The results of the other tests seem to show that the PDM holds the extrema a little bit better than FCT. This is clearly demonstrated in the cosine wave case where the maximum after 100 steps is 1.729 compared to 1.518 for FCT. Also, the typical three-point plateau for FCT appears, whereas PDM keeps the maximum at the right place. Each of the schemes has a tendency to form a plateau with more extension in the direction of the flow for a maximum and vice The choice of A = 0, B = 1 for the simple versa for a minima. scheme seems to have this tendency in far lesser degree. After transport over 20 meshpoints the cosine wave is practically symmetrical, but with about half the amplitude found for the Lax-Wendroff scheme.

III. Conclusions

A simple transport scheme has been demonstrated. It prevents the occurrence of new extrema (and therefore assures monatonicity). The additional donor cell contributions needed can be chosen according to the two parameters A and B. The most diffusive choice A = 0, B = 1, will result in a scheme slightly more diffuse than FCT, but it will guarantee the nonoccurrence of new extrema caused by the higher order scheme. Application of PDM in one dimension requires the same number of operations as FCT (for the ASC at NRL). It can readily be applied to nonsplit multidimensional problems.

Acknowledgements

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Appendix A

In this appendix a short description of the FCT algorithm actually used in the test runs is given. Theory and more details are given in ref. (1). Let H be the transport operator for one timestep (either the simple scheme (a) or the Lax-Wendroff scheme),

then

$$f_{j}^{H} = Hf_{j} \tag{A1}$$

if is the transported function. Now a diffused function \boldsymbol{f}^{DH} is computed using the old values

$$f_{j}^{DH} = f_{j}^{H} + 1/8 (df_{j+1/2} - df_{j-1/2})$$
 (A2)

in order to obtain the antidiffusive flux $\mathrm{df}_{j+1/2}^A$, it is useful to define a factor S by

$$s_{j+1/2} = sign (df_{j+1/2}) 1/2$$

(|sign (df_{j+3/2}) + sign (df_{j+1/2}) + sign (df_{j+1/2}) |-1)(A3)

which is 0 if the sign of the three differences are different. With the help of this factor, the antidiffusive flux is given by

$$df_{j+1/2}^{A} = S_{j+1/2} \quad min (|df_{j+3/2}^{DH}|, |df_{j-1/2}^{DH}|, 1/8|df_{j+1/2}|)$$
 (A4)

Then final resulting function is then given by

$$\hat{f}_{j} = f_{j}^{DH} - (df_{f+1/2}^{A} - df_{j-1/2}^{A})$$
 (A5)

Appendix B

Here a short description for the PDM scheme for variable velocities and grids are given. The choice of A=0, B=1 is incorporated. Results obtained in a multidimensional hydrocode applying PDM have been optimal with this choice.

Let H be the hydrooperator for one timestep

$$\mathbf{f}_{\mathbf{j}}^{\mathbf{H}} = \mathbf{H}\mathbf{f}_{\mathbf{j}} \tag{B1}$$

then $f_{\underline{j}}^{H}$ is the updated function.

The following formula can be applied in different directions in a onestep hydrocode by taking the appropriate differences. Be

$$S_j = 1/4 | sign (df_{j+1/2}) + sign (df_{j-1/2}) |$$
 (B2)

then S_j vanishes if the signs are different. It is 1/2 for the same signs. The diffusive flux $\dim_{j+1/2}$ is then given by

$$\begin{aligned} \text{dif}_{j+1/2} &= 1/2 \text{ dt } |\mathbf{u}_{j+1/2}| \text{ sign } (\text{df}_{j+1/2}) \text{ max } (0., |\text{df}_{j+1/2}| \\ &- (1 - \text{sign } (\mathbf{u}_{j+1/2})) \text{ S}_{j+1} |\text{df}_{j+3/2}| \\ &- (1 + \text{sign } (\mathbf{u}_{j+1/2})) \text{ S}_{j} |\text{df}_{j-1/2}| \end{aligned} \tag{B3}$$

Finally the new values f are given by

$$\hat{f}_{j} = f_{j}^{H} + (dif_{j+1/2} - dif_{j-1/2})/dx_{j+1/2}$$
 (B4)

	t =	2.0			t =	20.0			
Analy Value				6234160					
A B	1 2	0 1	FCT	A B	1 2	0 1	FCT		
						.012			
7200						.032			
0.0	0.000	.000	.000		.002	.077	.000		
0.0	.006	.039	.004		.040	.169	.004		
0.0	.247	.264	.246		.409	.339	.436		
1.0	.789	.745	.795		.733	.620	.739		
1.0	.963	.758	.964		.886	.847	.889		
1.0	.995	.996	.996		.955	.942	.956		
1.0	1.000	1.000	1.000		.984	.974	.984		
1.0	1.000	1.000	1.000		.995	.980	.995		
1.0	1.000	1.000	1.000		.998	.978	.998		
1.0	1.000	1.000	1.000		.998	.964	.998		
1.0	1.000	1.000	1.000		.997	.924	.998		
1.0	.994	.962	1.000		.959	.834	.996		
1.0	.753	.736	.754		.592	.663	.565		
0.0	.211	.255	.206		.268	.382	.261		
0.0	.037	.042	.036		.114	.159	.111		
0.0	.005	.005	.005		.045	.062	.044		
					.016	.023	.016		
					.006	.008	.006		
					.002	.002	.002		

TABLE 1.

10 Point Square Wave
Simple Method

	t = 2	2.0			<u>t =</u>	2.0	
Analytic Values							
A B	1.0	1.0	FCT	A B	1.0	0.0	FCT
0.0	.000	.000	.000		.003	.041	.000
0.0	.000	.000	.000		.092	.098	.062
0.0	.006	.038	.000		.331	.213	.265
0.0	.383	.315	.424		.424	.312	.349
1.0	.807	.684	.614		.432	.335	.363
1.0	.589	.631	.614		.386	.331	.363
0.0	.178	.281	.299		.194	.298	.339
0.0	.033	.046	.047		.084	.212	.159
0.0	.004	.005	.006		.034	.090	.063
0.0	.000	.000	.000		.013	.032	.023
0.0	.000	.000	.000		.004	.011	.008

TABLE 2

2-Point Square Wave

Simple Method

Analytic Values							
A B	2	0	FCT	A B	2	0 1	FCT
.000	.069	.132	.148		.274	.547	.482
.191	.125	.237	.148		.326	.639	.482
.691	.666	.612	.604		.940	.816	.849
1.309	1.460	1.345	1.485		1.504	1.180	1.363
1.809	1.864	1.814	1.810		1.700	1.381	1.503
2.000	1.931	1.868	1.852		1.726	1.403	1.518
1.809	1.875	1.763	1.852		1.674	1.361	1.518
1.309	1.334	1.389	1.396		1.060	1.184	1.151
.691	.541	.655	.515		.496	.820	.637
.191	.136	.186	.191		.300	.619	.497
.000	.069	.132	.148		.274	.597	.482

TABLE 3
Simple Method

	<u>t =</u>	2.0			<u>t</u> =	20.0	
Analyti Values	С						
A B	1.0	1.0	FCT	A B	0.0 4.0	0.0	FCT
0.0	.000	.000	.000		.000	.057	.000
0.0	.000	.000	.000		.007	.118	.000
0.0	.004	.047	.000		.140	.222	.192
0.0	.292	.289	.293		.468	.384	.470
1.0	.765	.731	.768		.679	.601	.680
1.0	.948	.943	.948		.822	.786	.823
1.0	.992	.992	.992		.409	.893	.911
1.0	.999	.999	1.000		.958	.943	.960
1.0	1.000	1.000	1.000		.982	.956	.982
1.0	1.000	1.000	1.000		.993	.955	.988
1.0	1.000	.000	1.000		.994	.935	.988
1.0	1.000	1.000	1.000		.998	.882	.988
1.0	1.000	1.958	1.000		.812	.781	.820
1.0	.708	.711	.707		.533	.619	.534
0.0	.235	.269	.232		.321	.401	.321
0.0	.052	.057	.052		.178	.220	.178
0.0	.008	.008	.008		.091	.112	.091
0.0	.000	.001	•000		.043	.053	.043

TABLE 4.

10-Point Square Wave

LW Method

Analytic Values		2.0			<u>t =</u>	20.0	Name of
A B	1.0	0.0	FCT	E	A 1.0 B 4.0	0.0	FCT
0.0	.000	.000	.000		.000	.028	.000
0.0	.000	.000	.000	1884	.009	.061	.010
0.0	.000	.000	.000		.153	.122	.138
0.0	.003	.047	.006		.298	.215	.248
0.0	.390	.335	.432	1.000	.368	.282	.303
1.0	.762	.659	.576		.378	.300	.314
1.0	.579	.604	.576	l ton	.331	.296	.314
0.0	.210	.285	.332		.214	.268	.300
0.0	.048	.060	.069		.125	.203	.186
0.0	.008	.009	.010		.067	.114	.000
0.0	.001	.001	.001		.033	.054	.050
0.0	.000	.000	.000		.015	.024	.023

TABLE 5.

2-Point Square Wave

LW Method

	t = :	2.0			<u>t</u>	= 20.0	
Analyti Values	.c						
A	1.0	0.0		A	1.0	0.0	
В	4.0	1.0	FCT	В	4.0	1.0	FCT
.000	.085	.157	.188		.409	.712	.665
.191	.175	.271	.188		.579	.753	.665
.691	.743	.655	.658		1.067	.894	.939
1.309	1.391	1.323	1.429		1.410	1.135	1.228
1.809	1.811	1.772	1.762		1.571	1.270	1.325
2.000	1.915	1.843	1.812		1.591	1.288	1.335
1.809	1.825	1.728	1.812		1.421	1.247	1.335
1.309	1.257	1.345	1.342	- 100	.934	1.105	1.061
.691	.603	.677	.571		.590	.865	.772
.191	.189	.229	.238		.429	.730	.674
.000	.085	.157	.188		.409	.712	.665

TABLE 6.

Lax-Wendroff Method